Pitchfork bifurcations in blood-cell shaped dipolar Bose-Einstein condensates

Stefan Rau, Jörg Main, Patrick Köberle, and Günter Wunner
Institut für Theoretische Physik 1, Universität Stuttgart, 70550 Stuttgart, Germany
(Dated: January 8, 2010)

We demonstrate that the method of coupled Gaussian wave packets is a full-fledged alternative to direct numerical solutions of the Gross-Pitaevskii equation of condensates with electromagnetically induced attractive $1/r$ interaction, or with dipole-dipole interaction. Moreover, Gaussian wave packets are superior in that they are capable of producing both stable and unstable stationary solutions, and thus of giving access to yet unexplored regions of the space of solutions of the Gross-Pitaevskii equation. We apply the method to clarify the theoretical nature of the collapse mechanism of blood-cell shaped dipolar condensates: On the route to collapse the condensate passes through a pitchfork bifurcation, where the ground state itself turns unstable, before it finally vanishes in a tangent bifurcation.

PACS numbers: 67.85.-d, 03.75.Hh, 05.30.Jp, 05.45.-a

arXiv:1001.1253v1 [cond-mat.quant-gas] 8 Jan 2010

Bose-Einstein condensates (BECs) with dipole-dipole interaction have become an active and exciting field of research because they offer the possibility of tuning the relative strengths of the short-range isotropic contact interaction and the anisotropic long-range dipole interaction by manipulating the s-wave scattering length via Feshbach resonances, and thus of studying a wealth of new phenomena that occur as one crosses the whole range from dominance of the contact interaction to that of the dipole interaction. The experimental realization of a BEC of chromium atoms [1–3], which possess a strong magnetic dipole moment, has given additional impetus to the field (for a comprehensive list of references see the recent review by Lahaye et al. [4]). In the dilute limit, the theoretical description of these condensates can be done in the framework of the Gross-Pitaevskii equation (GPE). This nonlinear Schrödinger equation has been solved in the literature so far by simple variational ansatzes, where the mean-field energy is minimized, e.g., with the conjugate gradient method or by imaginary time evolution. In this Letter we will show that the method of coupled Gaussian wave packets is an adequate alternative to solving the GPE of BECs with long-range interactions. Moreover, we will show that the method is superior in that it also yields unstable stationary solutions, and thus opens access to regions of the space of solutions of the GPE unexplored heretofore. As an application of the method we will analyze in detail the theoretical nature of the collapse mechanism of dipolar BECs.

The GPE for ultracold gases with long-range interactions, described by the interatomic potential $V_{\rm lr}(\boldsymbol{r})$, has the form

$$i\frac{\mathrm{d}}{\mathrm{d}t}\psi(\boldsymbol{r},t) = \big[-\Delta+\gamma_x^2x^2+\gamma_y^2y^2+\gamma_z^2z^2 +8\pi Na\,|\psi(\boldsymbol{r},t)|^2+V_{\rm lr}\,(\boldsymbol{r})\big]\psi(\boldsymbol{r},t)\,, \qquad (1)$$

where for dipolar interaction we have

$$V_{\rm lr}(\boldsymbol{r}) = N\int \mathrm{d}^3\boldsymbol{r'}\frac{1-3\cos^2\vartheta'}{|\boldsymbol{r}-\boldsymbol{r'}|^3}|\psi(\boldsymbol{r'},t)|^2. \qquad (2)$$

with ϑ' the angle between $\boldsymbol{r}-\boldsymbol{r'}$ and the axis of an external magnetic field. For completeness we will also consider the case of an isotropic "gravity-like" attractive $1/r$ long-range interaction,

$$V_{\rm lr}(\boldsymbol{r}) = -2N\int \mathrm{d}^3\boldsymbol{r'}\frac{|\psi(\boldsymbol{r'},t)|^2}{|\boldsymbol{r}-\boldsymbol{r'}|}\,. \qquad (3)$$

According to O'Dell et al. [5] this interaction could be electromagnetically induced by exposing the condensate atoms to an appropriately arranged set of triads of laser beams. The appealing feature of such "monopolar" condensates is that they can be self-trapping, i.e. exist without an external trapping potential. The equations above have been brought into dimensionless form by introducing natural units, which for monopolar interaction ($V_{\rm mono} = -u/r$) are [6–8] the "Bohr radius" $a_u = \hbar^2/(mu)$ for lengths, the "Rydberg energy" $E_u = \hbar^2/(2ma_u^2)$ for energies and $\omega_u = E_u/\hbar$ for frequencies. Natural units for dipolar atoms with magnetic moment μ are [9] the dipole length $a_{\rm d} = \mu_0\mu m/(2\pi\hbar^2)$, the dipole energy $E_{\rm d} = \hbar^2/(2ma_{\rm d}^2)$ and the dipole frequency $\omega_{\rm d} = E_{\rm d}/\hbar$. The quantities $\gamma_{x,y,z}$ in (1) denote the trapping frequencies in the three spatial directions measured in the respective frequency units, N is the number of bosons, and a the scattering length in units of a_u and $a_{\rm d}$, respectively.

The most obvious way of solving the Gross-Pitaevskii equation (1) is its direct numerical integration on multidimensional grids using, e.g., fast-Fourier techniques. The *stationary ground state* can be obtained by imaginary time evolution. These calculations, however, may turn out laborious, and physical insight can often be gained using approximate, in particular, variational solutions. A common approach employed for determining the dynamics and stability of condensates both with contact interaction only [10, 11] and with additional long-range interaction [8] is to assume a simple Gaussian form of the wave function, with time-dependent width parameters and phase, and to investigate the dynamics of these

quantities. For dipolar condensates improvements on the simple Gaussian form were made by multiplying it by second-order Hermite polynomials [12].

As an alternative to numerical quantum simulations on multidimensional grids we will extend the variational calculations in such a way that numerically converged results are obtained with significantly reduced computational effort compared to the exact quantum simulations but with similar accuracy. The method is that of *coupled Gaussian wave packets*. It was originally proposed by Heller [13, 14] to describe quantum dynamics in the semiclassical regime, and was successfully applied to the dynamics of molecules and atoms in external fields [15]. The idea is to choose trial wave functions which are *superpositions* of N different Gaussians centered at the origin

$$\psi(\boldsymbol{r},t) = \sum_{k=1}^{N} e^{i\left(a_x^k x^2 + a_y^k y^2 + a_z^k z^2 + \gamma^k\right)} \equiv \sum_{k=1}^{N} g^k(\boldsymbol{a}^k, \gamma^k; \boldsymbol{r}) \tag{4}$$

where both the width parameters $\boldsymbol{a}^k$ and the scalars γ^k are complex quantities, with the latter determining the weight and the phase of the individual Gaussian. Inserting the ansatz (4) into the time-dependent Gross-Pitaevskii equation and applying the time-dependent variational principle where $||i\dot{\Phi}(t) - H\psi(t)||^2$ is minimized by varying $\dot{\Phi}$, and afterwards $\dot{\Phi}$ is set equal to $\dot{\Phi} = \dot{\psi}$, yields a set of ordinary differential equations for the width parameters $\boldsymbol{a}^k$ and the scalars γ_k (cf. [15])

$$\dot{a}_\beta^k = -4(a_\beta^k)^2 - \frac{1}{2}V_{2,\beta}^k; \qquad \beta = x, y, z; \tag{5a}$$

$$\dot{\gamma}^k = 2i(a_x^k + a_y^k + a_z^k) - v_0^k. \tag{5b}$$

The quantities (v_0^k, V_2^k) with $k = 1, \ldots, N$ constitute the solution vector to the set of linear equations

$$\sum_{k=1}^{N} \left\langle g^l | x_\alpha^m x_\alpha^n v_0^k | g^k \right\rangle + \frac{1}{2}\sum_{k=1}^{N} \left\langle g^l | x_\alpha^m x_\alpha^n \mathbf{x} V_2^k \boldsymbol{x} | g^k \right\rangle = \sum_{k=1}^{N} \left\langle g^l | x_\alpha^m x_\alpha^n V(\boldsymbol{x}) | g^k \right\rangle \tag{6}$$

with $l = 1, \ldots, N$; $m + n = 0, 2$; and $x_1 = x$, $x_2 = y$, $x_3 = z$. Here, $V(\boldsymbol{x}) = V_\mathrm{c} + V_\mathrm{lr} + V_\mathrm{t}$ denotes the sum of the contact, the long-range and of external trap potentials. The important and appealing point of this procedure is that all necessary integrals with the trial wave functions g^l, g^k from (4) can be calculated analytically.

Stationary variational solutions to the extended Gross-Pitaevskii equation (1) are found by searching for the fixed points of (5), i.e. solving $\dot{\boldsymbol{a}}^k = 0; \dot{\gamma}^k = 0$ for each $k = 1, ..., N$ via a $4N$ dimensional highly nonlinear root search. The resulting stationary width and weight/phase parameters can then be used to calculate the mean field energy $E_\mathrm{mf} = \left\langle \Psi | -\Delta + V_\mathrm{t} + \frac{1}{2}(V_\mathrm{c} + V_\mathrm{lr}) | \Psi \right\rangle$ and the chemical potential $\mu = \left\langle \Psi | -\Delta + V_\mathrm{t} + V_\mathrm{c} + V_\mathrm{lr} | \Psi \right\rangle$. It is important to note that in contrast to numerical calculations with imaginary time evolution, which only work for stable solutions, this procedure will produce both stable and unstable solutions, and thus uncover yet unexplored parts of the space of solutions of the Gross-Pitaevskii equation.

To analyze the stability of the stationary solutions the dynamical equations (5) are split into real (R) and imaginary (I) parts and linearized around the fixed points. The eigenvalues of the Jacobian matrix $\mathbf{J}$ at the fixed point

$$\boldsymbol{J} = \frac{\partial\left(\dot{a}_\alpha^{k,R}, \dot{a}_\alpha^{k,I}, \dot{\gamma}^{k,R}, \dot{\gamma}^{k,I}\right)}{\partial\left(a_\beta^{l,R}, a_\beta^{l,I}, \gamma^{l,R}, \gamma^{l,I}\right)}, \tag{7}$$

with $\alpha, \beta = x, y, z$; $k, l = 1, ..., N$, determine the stability properties of the solution. If all eigenvalues λ_j of the system are purely imaginary, the motion is confined to the vicinity of the fixed point and quasi-periodic. If one real part or several real parts of the eigenvalues are non-zero, small variations from the fixed point lead to exponential growth of the perturbation.

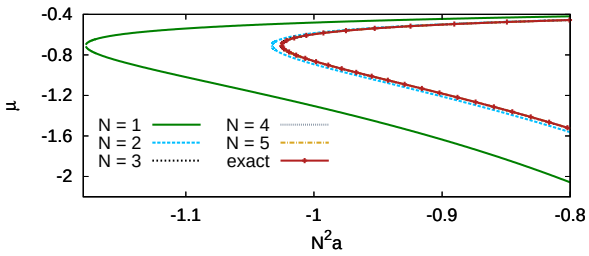

FIG. 1: Chemical potential μ for self-trapped condensates with attractive $1/r$ interaction as a function of the scaled scattering length N^2a obtained by using up to 5 Gaussian wave packets in comparison with the result of the exact numerical solution of the stationary Gross-Pitaevskii equation. Note that all forms yield a tangential bifurcation diagram, with a stable (upper) and an unstable (lower) branch. The inclusion of three Gaussians already well reproduces the exact numerical result.

As a first application we demonstrate the efficiency of the coupled Gaussian wave packet method for condensates with attractive $1/r$ long-range interaction, for the case of self-trapping ($\gamma_{x,y,z} = 0$). Figure 1 shows the results for the chemical potential as a function of the scaled scattering length N^2a for superpositions of 1 to 5 Gaussians in comparison with the results of the exact numerical solution. It is evident that all forms reproduce the bifurcation behavior discussed in [6–8]: at a critical point two solutions of the Gross-Pitaevskii equation are born in a tangent bifurcation, one stable (upper branch) and one unstable (lower branch). The numerically accurate bifurcation point lies at $a_\mathrm{cr} \approx -1.025147$. It can also be seen that, while the variational calculation with one Gaussian, with $a_\mathrm{cr}^{\mathrm{N}=1} = -1.178$, still lies far off the

correct result, the inclusion of only one more Gaussian brings the chemical potential curve already close to the numerical result, and practically no improvement is visible in Fig. 1 when 3 or more Gaussians are included. Using 5 coupled Gaussians the exact bifurcation point is reproduced with an accuracy of 10^{-6}. Similar results are obtained in the presence of a trapping potential.

We now turn to dipolar condensates. Previous studies [12, 16] have shown that in certain regions of the parameter space dipolar condensates assume a non-Gaussian biconcave "blood-cell-like" shape. To demonstrate the power of the coupled Gaussian wave packet method, we choose a set of such parameters. We consider an axisymmetric trap with (particle number scaled) trap frequencies $N^2\gamma_z = 25200$ along the polarization direction of the dipoles and $N^2\gamma_\rho = 3600$ in the plane perpendicular to it (corresponding to an aspect ratio of $\lambda = \gamma_z/\gamma_\rho = 7$). For this set of parameters we show in Fig. 2 (a) the

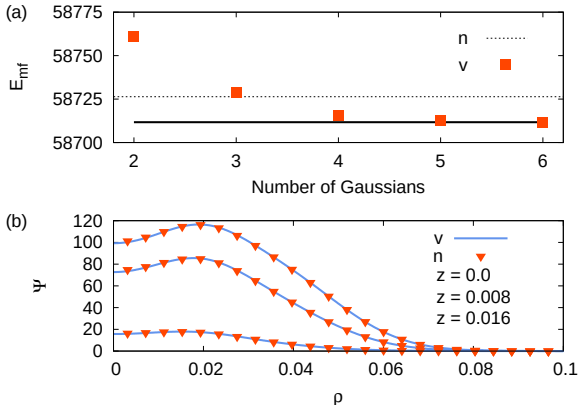

FIG. 2: (a) Convergence of the mean-field energy with increasing number of coupled Gaussian wave packets (squares) and comparison with the value obtained by a lattice calculation with grid size 128×512 (dashed line), which lies energetically higher than the exact converged variational solution (solid line). (b) Comparison of the variational wave function for 6 coupled Gaussians (solid curves) with values of the numerical one (triangles) at different z coordinates. Both solutions show a biconcave shaped condensate. The figures are for (particle number scaled) trap frequencies $N^2\gamma_z = 25200$ and $N^2\gamma_\rho = 3600$, and scattering length $a = 0$.

convergence behavior of the mean field energy. We compare the variational solution as the number of Gaussian wave packets is increased from 2 to 6 with the mean field energy value of a numerical lattice calculation (imaginary time evolution combined with FFT) with a grid size of 128×512, at scattering length $a = 0$ as an example. The mean field energy for one Gaussian is $E_{\rm mf} = 60361\, E_{\rm d}$ and lies far outside the vertical energy scale. Evidently the numerical value is more than excellently reproduced by 5 and 6 coupled Gaussians. The behavior for other scattering lengths is similar. Also the wave function nicely converges, and moreover, as can be seen in Fig. 2 (b), reproduces the biconcave shape of the condensate as does the numerical solution. Thus the method of coupled Gaussians is a viable and full-fledged alternative to direct numerical solutions of the Gross-Pitaevskii equation for dipolar condensates.

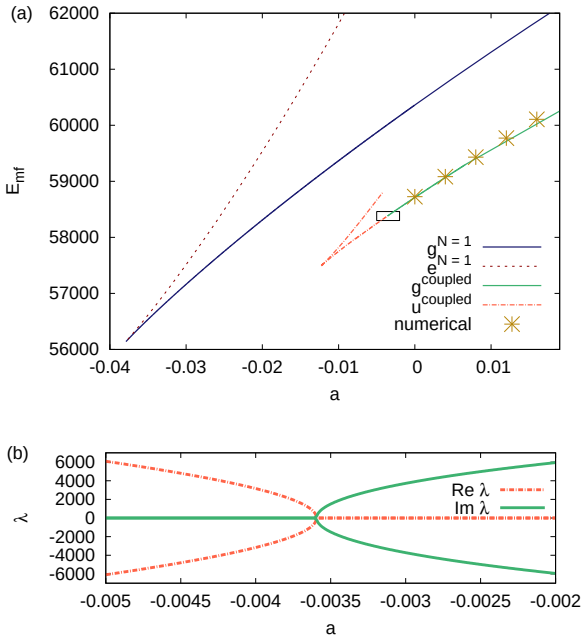

FIG. 3: (a) Mean field energy of a dipolar condensate for (particle number scaled) trap frequencies $N^2\gamma_z = 25200$ and $N^2\gamma_\rho = 3600$ as a function of the scattering length. In the variational calculation with one Gaussian a stable ground state ($g^{N=1}$) and an unstable excited state ($e^{N=1}$) emerge in a tangent bifurcation. Using coupled Gaussians two unstable states emerge (labeled $u^{\rm coupled}$), of which the lower one turns into a stable ground state ($g^{\rm coupled}$) in a pitchfork bifurcation. (b) Stability eigenvalues λ of the pitchfork bifurcation point for calculations with 6 coupled Gaussians, scattering length in rectangle marked in (a). Real and imaginary parts of two selected eigenvalues of the Jacobian (7) as a function of the scattering length. For $a < a_{\rm cr}^{\rm p} = -0.00359$ the solution is unstable with one pair of real eigenvalues. At $a_{\rm cr}^{\rm p}$ the real eigenvalues vanish in a pitchfork bifurcation and a stable ground state forms with purely imaginary eigenvalues. Only those eigenvalues involved in the stability change are shown.

Figure 3 (a) shows, for the same set of trap frequencies, the results for the mean field energy of the condensate as a function of the scattering length a (in units a_d) for a wave function with one Gaussian, and for 5 coupled Gaussian wave packets. Results obtained using 6 Gaussians would be indistinguishable in the figure from those obtained using 5 Gaussians, and the results for 2–4 Gaussians are not shown for the sake of clarity of the figure.

Similar to the above findings for monopolar condensates, and as is known from previous variational calculations [9] for dipolar condensates, for $N = 1$ two branches of solution are born in a tangent bifurcation. The en-

ergetically higher branch has purely real stability eigenvalues $\pm\lambda^R$, corresponding to an unstable excited state $\mathrm{e}^{\mathrm{N=1}}$, the lower branch possesses purely imaginary eigenvalues $\pm\lambda^I$ and corresponds to the stable ground state $\mathrm{g}^{\mathrm{N=1}}$. At the bifurcation point the branches of the stability eigenvalues merge and vanish.

The situation is different if the condensate wave function is described by more than one Gaussian. As the scattering length is decreased from positive values towards the tangent bifurcation, the branch corresponding to the ground state $\mathrm{g}^{\mathrm{coupled}}$ turns into an unstable state $\mathrm{u}^{\mathrm{coupled}}$ at a scattering length of $a_{\mathrm{cr}}^{\mathrm{p}} = -0.00359$. This is evident from the stability analysis shown in Fig. 3 (b) where the stability eigenvalues for the ground state, calculated using 6 Gaussians, are plotted in a small interval of the scattering length around $a_{\mathrm{cr}}^{\mathrm{p}}$. Above $a_{\mathrm{cr}}^{\mathrm{p}}$ the eigenvalues are purely imaginary, below they are purely real. [Note that in a Bogoliubov analysis this instability should appear as a dynamical instability.] The ground state remains unstable down to the tangent bifurcation point at $a_{\mathrm{cr}}^{\mathrm{t}} = -0.01224$, where it joins the branch of the unstable excited state.

The quality of the calculation using 5 Gaussian wave packets is also demonstrated in Fig. 3 (a) where the results of a numerically grid calculation by imaginary time evolution are shown by crosses. Evidently the numerical results and the results obtained using 5 coupled Gaussians excellently agree. The imaginary time calculation, however, can only trace the stable branch of the solution and fails for the unstable branch. Thus it is demonstrated that the Gaussian wave packet method is not only numerically accurate but also capable of giving access to regions of the space of solutions of the Gross-Pitaevskii equation with dipolar interaction that are difficult to investigate by conventional numerical full quantum calculations.

The phenomenon of one smooth branch of solutions becoming unstable as a function of a control parameter is reminiscent of a *pitchfork* bifurcation. The two stable solutions on the fork arms which should also be born in a pitchfork bifurcation, and exist in a tiny neighborhood $(a_{\mathrm{cr}}^{\mathrm{p}} - \epsilon) < a < a_{\mathrm{cr}}^{\mathrm{p}}$, are numerically hard to trace and therefore not plotted in the figure. Their existence, and the pitchfork type of the bifurcation, however, can be proven by looking at the "phase portrait" plotted in Fig. 4 at a value of the scattering length $a = -0.036$ slightly below $a_{\mathrm{cr}}^{\mathrm{p}}$. Figure 4 shows contours of equal deviation of the mean field energy from that of the ground state in the plane spanned by the two eigenvectors whose eigenvalues are involved in the stability change in Fig 3 (b). The coordinate axes δ_1, δ_2 correspond to small variations of the Gaussian parameters in the eigenvector directions around the hyperbolic fixed point solution located at the origin. The portrait clearly reveals the existence of two nearby elliptic fixed points corresponding to two additional stable solutions. Therefore, in a small interval ϵ of the scattering length below $a_{\mathrm{cr}}^{\mathrm{p}}$, $(a_{\mathrm{cr}}^{\mathrm{p}} - \epsilon) < a < a_{\mathrm{cr}}^{\mathrm{p}}$, there exist two additional branches, besides the unstable solution. This proves that the bifurcation is of pitchfork type. Note that the classification of the condensate as unstable for $a < a_{\mathrm{cr}}^{\mathrm{p}}$ nevertheless remains true in physical terms due to the numerically small value of ϵ. We also note that for $a > a_{\mathrm{cr}}^{\mathrm{p}}$ the phase portrait possesses only one elliptic fixed point cooresponding to the stable stationary ground state.

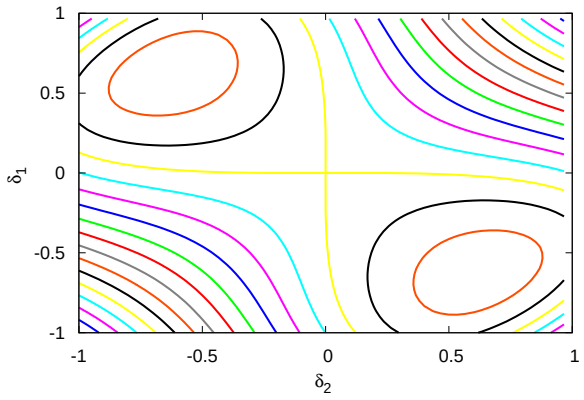

FIG. 4: Contour plot of the mean field energy with the eigenvectors corresponding to the eigenvalues of Fig. 3 (b) linearizing the vicinity of the fixed point (δ_1, δ_2 in arbitrary units). The figure shows $a = -0.0036$ close below the pitchfork bifurcation point, showing three fixed points: Two stable and one hyperbolic.

Is there a chance of observing dipolar BECs on the stable fork arms? The answer probably is no, in the same way as it is in the case of the question of observing the transition to structured ground states, possibly associated with a roton instability, shortly before collapse. The reason is the difficulty of adjusting trap frequencies and the scattering length to the necessary precision in a real experiment. Nevertheless theoretical investigations of this type close to the threshold of instability of dipolar condensates are valuable in their own right since they help to understand the nature of the collapse, and thus of "what's really going on".

[1] A. Griesmaier, J. Werner, S. Hensler, J. Stuhler, and T. Pfau, Phys. Rev. Lett. **94**, 160401 (2005).

[2] J. Stuhler, A. Griesmaier, T. Koch, M. Fattori, T. Pfau, S. Giovanazzi, P. Pedri, and L. Santos, Phys. Rev. Lett. **95**, 150406 (2005).

[3] Q. Beaufils, R. Chicireanu, T. Zanon, B. Laburthe-Tolra, E. Maréchal, L. Vernac, J.-C. Keller, and O. Gorceix, Phys. Rev. A **77**, 061601(R) (2008).

[4] T. Lahaye, C. Menotti, L. Santos, M. Lewenstein, and T. Pfau, Rep. Prog. Phys. **72**, 126401 (2009).

[5] D. O'Dell, S. Giovanazzi, G. Kurizki, and V. M. Akulin, Phys. Rev. Lett. **84**, 5687 (2000).

[6] I. Papadopoulos, P. Wagner, G. Wunner, and J. Main, Phys. Rev. A **76**, 053604 (2007).
[7] H. Cartarius, J. Main, and G. Wunner, Phys. Rev. A **77**, 013618 (2008).
[8] H. Cartarius, T. Fabčič, J. Main, and G. Wunner, Phys. Rev. A **78**, 013615 (2008).
[9] P. Köberle, H. Cartarius, T. Fabčič, J. Main, and G. Wunner, New Journal of Physics **11**, 023017 (2009).
[10] V. M. Pérez-García, H. Michinel, J. I. Cirac, M. Lewenstein, and P. Zoller, Phys. Rev. Lett. **77**, 5320 (1996).
[11] V. M. Pérez-García, H. Michinel, J. I. Cirac, M. Lewenstein, and P. Zoller, Phys. Rev. A **56**, 1424 (1997).
[12] S. Ronen, D. C. E. Bortolotti, and J. L. Bohn, Phys. Rev. Lett. **98**, 030406 (2007).
[13] E. J. Heller, J. Chem. Phys. **65**, 4979 (1976).
[14] E. J. Heller, J. Chem. Phys. **75**, 2923 (1981).
[15] T. Fabčič, J. Main, and G. Wunner, Phys. Rev. A **79**, 043416 and 043417 (2009).
[16] O. Dutta and P. Meystre, Phys. Rev. A **75**, 053604 (2007).